

**HIGH PRODUCTION VOLUME (HPV)  
CHEMICAL CHALLENGE PROGRAM**

**TEST PLAN**

**For**

**4,4'-oxydibenzenesulfonohydrazide,**

**CAS No. 80-51-3**

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**Submitted to the US EPA**

**By**

**Crompton Corporation**

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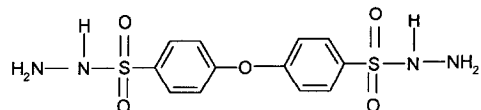
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## 1. General Information

1.1 CAS Number: 80-51-3

1.2 Molecular Weight: 358.39

1.3 Structure and formula: C<sub>12</sub>H<sub>14</sub>N<sub>4</sub>O<sub>5</sub>S<sub>2</sub>



## 1.4 Introduction

4,4'-oxydibenzenesulfonohydrazide is used as a chemical blowing agent in the manufacture of foam rubber and plastic products.

## 2. Review of Existing Data and Development of Test Plan

Crompton Corporation has undertaken a comprehensive evaluation of all relevant data on the SIDS endpoints of concern for Celogen OT. The availability of the data on the specific SIDS endpoints is summarized in Table 1. Table 1 also shows data gaps that will be filled by additional testing.

Table 1: Available adequate data and proposed testing for 4,4'-oxydibenzenesulfonohydrazide

CAS No. 80-51-3	Information Available?	GLP	OECD Study?	Other Study?	Estimation Method?	Acceptable?	SIDS Testing required?
	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
<b>Physicochemical</b>							
Melting Point	Y	N			N	Y	N
Boiling Point	Y	N			N	Y	N
Vapour Pressure	Y	N			Y	Y	N
Water Solubility	Y	N			Y	Y	N
Partition Coefficient (Kow)	Y	N			Y	Y	N
<b>Environmental Fate</b>							
Biodegradation	Y				Y	Y	N
Hydrolysis	N						N
Photodegradation	Y				Y	Y	N
Transport and Distribution between Environmental Compartments	Y				Y	Y	N
<b>Ecotoxicology</b>							
Acute Fish	Y				Y	Y	N
Acute Daphnia	Y				Y	Y	N
Acute Algae	Y				Y	Y	N
<b>Toxicology</b>							
Acute Oral	Y	N		Y		Y	N
Repeat Dose toxicity	Y	N			N	Y	N
Genetic toxicity – Gene mutation	Y	N			N	Y	N
Genetic toxicity – Chromosome aberration	Y				N	Y	N
Reproductive toxicity	N						Y
Developmental toxicity/teratogenicity	N						Y

**A. Evaluation of Existing Physicochemical Data and Proposed Testing**

1. Melting Point

It is reported in a peer-reviewed publication that 4,4'-oxydibenzenesulfonohydrazide begins to decompose at 150-160°C prior to melting.

2. Boiling Point

The boiling point of 4,4'-oxydibenzenesulfonohydrazide cannot be measured as the substance decomposes prior to melting.

3. Vapour Pressure

The vapour pressure of 4,4'-oxydibenzenesulfonohydrazide was calculated to be  $8.9 \times 10^{-12}$  hPa at 25°C using MPBPWIN v1.40.

4. Water Solubility

The water solubility of 4,4'-oxydibenzenesulfonohydrazide was calculated to be 4733 mg/L at 25°C using WSKOW v1.40.

5. Partition Coefficient

The log Pow of 4,4'-oxydibenzenesulfonohydrazide was estimated to be 0.08 using KOWWIN v1.66.

**Summary of Physicochemical Properties Testing: Existing data for melting point, boiling point, vapour pressure, water solubility and partition coefficient are considered to fill these endpoints adequately and, therefore, no further testing is planned.**

**B. Evaluation of Existing Environmental Fate Data and Proposed Testing**

1. Biodegradation

The biodegradation of 4,4'-oxydibenzenesulfonohydrazide has been estimated using Biowin v4.00 and the results predict the substance is not readily biodegradable.

2. Hydrolysis

There are no hydrolysable groups in the chemical structure, and the substance is therefore predicted to be hydrolytically stable.

3. Photodegradation

The potential for photodegradation of 4,4'-oxydibenzenesulfonohydrazide has been estimated using AOPWIN v1.90, and indicated atmospheric oxidation via OH radicals reaction with a half-life of 61 hours.

4. Transport and Distribution between Environmental Compartments

An Epiwin Level III Fugacity Model calculation has been conducted for 4,4'-oxydibenzenesulfonohydrazide and indicates even distribution between soil and water for emissions of 1000 kg/hr simultaneously to air, water and soil compartments.

**Summary of Environmental Fate Testing: Existing data for photodegradation and transport and distribution between environmental compartments are considered to fill these endpoints adequately. 4,4'-oxydibenzenesulfonylhydrazide contains no hydrolysable or biodegradable groups, therefore no hydrolysis or biodegradation testing is proposed.**

**C. Evaluation of Existing Ecotoxicity Data and Proposed Testing**

1. Acute Toxicity to Fish

Estimation using ECOSAR v0.99g gives an LC<sub>50</sub> (96 h) of 9.76 mg/L.

2. Acute Toxicity to Algae

Estimation using ECOSAR v0.99g gives an LC<sub>50</sub> (144 h) of 2.36 mg/L.

3. Acute Toxicity to Daphnia

Estimation using ECOSAR v0.99g gives an LC<sub>50</sub> (48 h) of 17.37 mg/L.

**Summary of Ecotoxicity Testing: 4,4'-oxydibenzenesulfonylhydrazide belongs to the Ecosar class of hydrazines. The predicted values for acute toxicity to fish, daphnia and algae are regarded as being valid for this material and no testing is proposed.**

**D. Evaluation of Existing Human Health Effects Data and Proposed Testing**

1. Acute Toxicity

The acute oral toxicity has been determined to be > 5200 mg/kg b.w. The acute dermal toxicity has been determined to be > 200 mg/kg b.w. (FIFRA Section 162.8(c)). When administered by interperitoneal injection, a LD<sub>50</sub> >5000 mg/kg b.w. was observed.

2. Skin Irritation

This non-SIDS endpoint has been evaluated for Celogen OT. Slight irritation occurred in rabbits treated with an aqueous extract of the chemical.

3. Repeat Dose Toxicity

Two repeat dose toxicity studies are reported in the literature. In the first of these a NOEL of 1mg/kg bw/day (90 day, oral feed, rat) was reported. In the second study a LOAEL of 36 mg/kg/day (4 month, gavage, rat) was reported.

4. Genotoxicity

The substance was mutagenic in the Ames test (*S. typhimurium*) with and without metabolic activation and also with one strain of *Escherichia coli* with metabolic activation. With other strains of *E. coli*, the substance was found to be non-mutagenic with or without metabolic activation. The substance gave negative results in a chromosome aberration study using human lymphocytes. It also gave negative results in a micronucleus assay and UDS assay.

5. Reproductive and Developmental Toxicity

The developmental and reproductive toxicity of Celogen OT in the rat will be determined using OECD Method 421.

**Summary of Human Health Effects Testing: The endpoints for developmental toxicity and reproductive toxicity (OECD 421) will be determined. The other human health endpoints have been filled adequately.**

**3. Evaluation of Data for Quality and Acceptability**

The collected data were reviewed for quality and acceptability following the general US EPA guidance [2] and the systematic approach described by Klimisch et al [3]. These methods include consideration of the reliability, relevance and adequacy of the data in evaluating their usefulness for hazard assessment purposes. This scoring system was only applied to ecotoxicology and human health endpoint studies per EPA recommendation [4]. The

codification described by Klimisch specifies four categories of reliability for describing data adequacy. These are:

- (1) **Reliable without restriction:** Includes studies or data complying with Good Laboratory Practice (GLP) procedures, or with valid and/or internationally accepted testing guidelines, or in which the test parameters are documented and comparable to these guidelines.
- (2) **Reliable with Restrictions:** Includes studies or data in which test parameters are documented but vary slightly from testing guidelines.
- (3) **Not Reliable:** Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.
- (4) **Not Assignable:** Includes studies or data in which insufficient detail is reported to assign a rating, e.g. listed in abstracts or secondary literature.

#### **4. References**

- [1] US EPA, EPI Suite Software, 2000
- [2] USEPA (1998). Guidance for Meeting the SIDS Requirements (The SIDS Guide). Guidance for the HPV Challenge Program. Dated 11/2/98.
- [3] Klimisch, H.-J., et al (1997). A Systematic Approach for Evaluating the Quality of Experimental Toxicological and Ecotoxicological Data. Regul. Toxicol. Pharmacol. 25:1-5
- [4] USEPA (1999). Determining the Adequacy of Existing Data. Guidance for the HPV Challenge Program. Draft dated 2/10/99.